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History and future perspectives of the Monte Carlo shell model -from Alphleet to K computer-

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Abstract. We report a history of the developments of the Monte Carlo shell model (MCSM). The MCSM was proposed in order to perform large-scale shell-model calculations which direct diagonalization method cannot reach. Since 1999 PC clusters were introduced for parallel computation of the MCSM. Since 2011 we participated the High Performance Computing Infrastructure Strategic Program and developed a new MCSM code for current massively parallel computers such as K computer. We discuss future perspectives concerning a new framework and parallel computation of the MCSM by incorporating conjugate gradient method and energy-variance extrapolation.

1. Introduction

The nuclear shell model calculation has been very successful in understanding the nuclear structure on the basis of nucleons interacting via the nuclear force. It can provide precisely the properties, excitation schemes and transition probabilities of the low-lying states of a nucleus. The conventional, standard solver for shell-model calculations is the exact diagonalization of Hamiltonian matrix by the Lanczos algorithm in a given model space. However, the dimension of the matrix grows exponentially as the number of valence nucleons increases and surpasses the numerical feasibility limit of the Lanczos method (e.g. 5×10^{15} for ^{68}Ni in $pfg9d5$-shell, discussed in Ref.[1]). In order to perform such large-scale shell model calculations, we have developed the Monte Carlo shell model (MCSM) method. The MCSM was firstly proposed by a part of the authors (M. Honma, T. Mizusaki and T. Otsuka) in 1995 [2], and has been developed by the nuclear theory group of the University of Tokyo. Since the MCSM algorithm is suited for parallel computations, we started the large-scale nuclear structure calculation project with introducing PC clusters since 1999. In the proceedings, we briefly report a history of the MCSM and utilization of PC clusters for parallel computations in view of computational aspect in Sect.2, and summarize the framework of the MCSM in Sect.3, the details of which can be

found in Ref.[3].

2. Computational aspects of the MCSM, Alphleet cluster and K computer

In 1999, a research project for large-scale shell-model calculations was launched jointly by the RIKEN Accelerator Research Facility (currently known as RIKEN Nishina center) and the nuclear theory group of the University of Tokyo. Since the MCSM calculation is suitable for parallel computation, we introduced a PC cluster, Alphleet-1, mainly for the MCSM calculations. It consisted of 73 workstations, each of which had 2 Alpha ev6 CPUs and was connected with each other by Myrinet network [4, 5]. A photograph of the system is shown in the left of Fig.1. The total system performance of LINPACK benchmark was 62GFLOPs, which was ranked as the 169th fastest computer in the world at Nov. 1999 [6]. The main achievements of this project were summarized in Ref.[7]. Especially, this project played an essential role to establish the effective interaction of pf shell, GXPF1 [8].

After the completion of the project with Alphleet-1 cluster, a succeeding joint project has started since the year 2001 based on a collaboration agreement between Center for Nuclear Study, the University of Tokyo (CNS) and RIKEN Nishina Center. In this project, PC clusters are provided by KAKENHI grants [9] through the Department of Physics, the University of Tokyo, but infrastructures (e.g. electricity, cooling, etc.) and running costs are supported primarily by CNS and RIKEN Nishina Center. Under this project, we introduced a computer cluster named Alphleet-2, which was comprised of 176 Alpha CPUs from 2001 to 2003. Its photo is shown in the right of Fig.1. Four racks on the right end of the photo were added in 2003 and were comprised of 64 CPUs and 128 GB main memory. Each computation node of the cluster are connected with each other via Myrinet network and has no hard disk drive. The features of these clusters are summarized in Tab.1. This project has been continued at present. Especially in 2012, we introduced a PC server equipped with 40 Intel Xeon cores and 660GB main memory mainly for conventional shell-model calculations with the Lanczos method.

Table 1. Features of Alphleet-1 and Alphleet-2.

	Fiscal Year	Brand name	Memory	Nodes
Alphleet-1	1999	DEC DS-20 (Alpha 2 CPUs)	512MB	73
Alphleet-2	2001	Compaq ES-45 (Alpha 4 CPUs)	16GB	28
	2003	Hewlett-Packard GS-1280 (Alpha 32 CPUs)	64GB	2

However, the number of processing units of the state-of-the-art massively parallel computers surpasses ten thousands, which cannot be caught up by a PC cluster of a local research group. In 2009, we decided to write a new MCSM code from scratch so that the MCSM calculations can be run on recent massively parallel computers. This new code was equipped with many advantages: hybrid parallel with Message Passing Interface library and OpenMP, capability of isospin-breaking interaction, applicability to *no-core* shell model calculations, and a new efficient algorithm for the computation of Slater determinants [10]. This new code played an essential role to develop a new framework of the MCSM utilizing the energy-variance extrapolation [17], which is discussed in Sect.3.2.

Based on these experiences of parallel computations of the MCSM and its achievements, we have participated in activities of High Performance Computing Infrastructure Strategic Programs for Innovative Research (SPIRE) Field 5 "The origin of matter and the universe" since 2011. The SPIRE project aims at an integral understanding of the origin and structure of matter and the Universe utilizing the K computer, which is the world's fastest supercomputer in 2011 [11]. In this project, we are in charge of the elucidation of nuclear properties by ultra

large-scale simulations of quantum many-body systems. In 2011, we carried out benchmark tests and performance tuning of the MCSM code at K computer.

3. Theoretical developments of the MCSM method

The major features of the recently developed MCSM framework are the variational procedure to obtain the approximated wave function, which is described in Sect.3.1, and the energy-variance extrapolation, which is described in Sect. 3.2.

3.1. Variational procedure

In the framework of the MCSM, the shell-model wave function is approximated as a linear combination of angular-momentum- and parity-projected Slater determinants,

$$|\Psi_{N_b}\rangle = \sum_{n=1}^{N_b} \sum_{K=-I}^{I} f_{n,K}^{(N_b)} P_{MK}^{I\pi} |\phi_n\rangle, \tag{1}$$

where N_b is the number of the Slater-determinant basis states. The $P_{MK}^{I\pi}$ operator is the angular-momentum and parity projector defined as

$$P_{MK}^{I\pi} = \frac{1+\pi\Pi}{2} \frac{2I+1}{8\pi^2} \int d\Omega \; {D_{MK}^{I}}^{*}(\Omega) e^{i\alpha J_z} e^{i\beta J_y} e^{i\gamma J_z}, \tag{2}$$

where $\Omega \equiv (\alpha, \beta, \gamma)$ are the Euler angles and $D_{MK}^{I}(\Omega)$ denotes Wigner's D-function. Π stands for the parity transformation. Each $|\phi_n\rangle$ is a deformed Slater determinant defined as

$$|\phi\rangle = \prod_{k=1}^{N_\mathrm{f}} \left(\sum_{l=1}^{N_\mathrm{sp}} D_{lk} c_l^\dagger \right) |-\rangle, \tag{3}$$

which is parametrized by the complex $N_\mathrm{sp} \times N_\mathrm{f}$ matrix D. N_f and N_sp are the numbers of fermions and single-particle states, respectively. The $|-\rangle$ denotes an inert core in the conventional shell-model calculations or the vacuum in no-core shell-model calculations.

The coefficients $f_{n,K}^{(N_b)}$ are determined by the diagonalization of the Hamiltonian matrix in the subspace spanned by the projected Slater determinants, $P_{MK}^{I\pi}|\phi_n\rangle$ with $-I \le K \le I$ and $1 \le n \le N_b$. This diagonalization also determines the energy, $E_{N_b} \equiv \langle \Psi_{N_b} | H | \Psi_{N_b} \rangle$, as a function of N_b. In the early stage of the development of the MCSM, the wave function is a linear combination of Slater determinants without angular-momentum projection, or only with z-component of the angular-momentum projection [12]. We increase N_b until E_{N_b} converges enough, or the extrapolated energy converges.

In the original MCSM calculation, the Slater determinant basis, $|\phi_n\rangle$, are selected from many candidates generated stochastically utilizing the auxiliary-field Monte Carlo technique, the detail of which is summarized in Ref. [7]. Recently, we have introduced an additional procedure, named sequential conjugate gradient (SCG) process, to obtain better basis states [13]. In this procedure we determine $D^{(n)}$ variationally to minimize $E_{N_b=n}$ utilizing the conjugate gradient method.

Here, we demonstrate how the original MCSM and the additional SCG process work with ^{56}Ni in the pf shell as an example. The effective interaction is taken as FPD6 interaction [14]. Its M-scheme dimension is 1,084,455,228, which is tractable by recent shell model codes with the Lanczos method [15]. At the time of the Alphleet-1 project, it was far beyond the limitation of the Lanczos method, and the MCSM enabled us to discuss the shape co-existence of ^{56}Ni. Since ^{56}Ni has been studied further by shell model calculations [16], it should be a good example for a benchmark test.

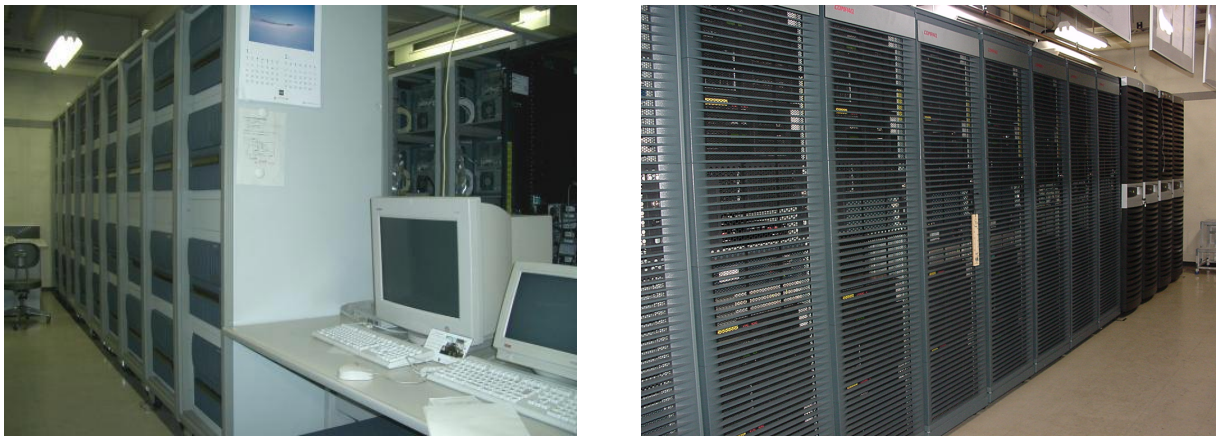

Figure 1. Left: Alphleet-1. Right: Alphleet-2.

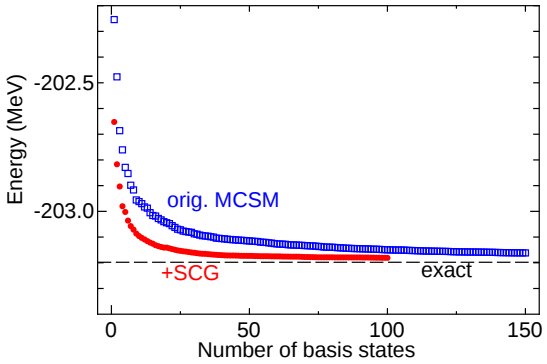

Figure 2. Energy convergence for the ground state of ^{56}Ni. against number of basis states. The blue open squares and red filled circles denote the result of the original MCSM and that of the SCG method, respectively.

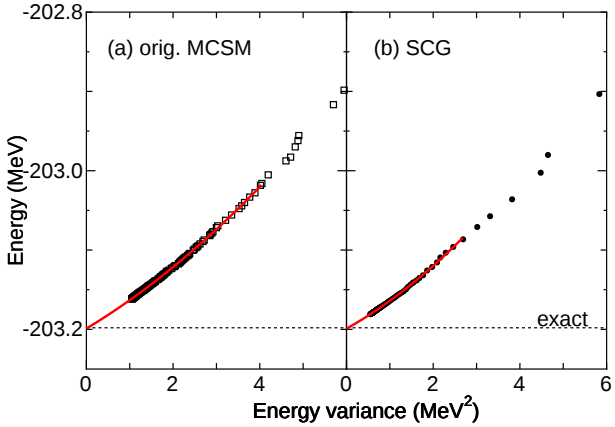

Figure 3. Energy and energy variance of the wave functions provided by (a) the original MCSM, and (b) SCG method for ^{56}Ni. The red lines are fitted for the points. The dashed line denotes the exact shell-model energy. See text for details.

Figure 2 shows that the energy expectation values of the MCSM wave function generated by two kinds of methods converge to the exact shell-model energy with increasing a number of basis states, N_b. The energy of the SCG is much better convergence than that of the original MCSM method. While the exact shell-model energy is -203.198MeV, that of the original MCSM is -201.161MeV with 150 basis states. The same energy (-201.161MeV) is reached by the SCG method with only 30 basis states. The energy of the SCG finally reaches -201.180MeV with 100 basis states. Nevertheless, the small gap between the SCG energy and the exact one, 18keV, remains. In order to remove this gap, we introduced the energy-variance extrapolation, which enables us to estimate the exact eigenvalue precisely even in case the Lanczos method cannot be applied [17].

3.2. Energy variance extrapolation method

The energy-variance extrapolation method is based on the fact that the energy variance of the exact eigenstate is zero. The energy variance of the approximated wave function is not exactly zero, but rather small and approaches zero as the approximation is improved. In the framework of the energy-variance extrapolation, we draw the energy $E_{N_b} = \langle\Psi_{N_b}|H|\Psi_{N_b}\rangle$ against the energy variance $\langle\Delta H^2\rangle_{N_b} = \langle\Psi_{N_b}|H^2|\Psi_{N_b}\rangle - E^2_{N_b}$. The variance usually approaches zero as N_b increases, and the point in the energy-variance plot approaches the y-axis. These points are fitted by a first- or second-order polynomial such as

$$E = c_0 + c_1\langle\Delta H^2\rangle + c_2(\langle\Delta H^2\rangle)^2, \tag{4}$$

where these coefficients c_0, c_1, and c_2 are determined by a least square fit. By extrapolating the fitted curve into the y-intercept we obtain the extrapolated energy, namely, c_0.

The variational procedure discussed in Sect. 3.1 provides us with a successive sequence of the wave functions, $|\Psi_{N_b}\rangle$ with $1 \le N_b \le N_m$, where N_m is the maximum of N_b. This sequence is utilized in the energy-variance extrapolation method. In practice we evaluate the energy E_{N_b} and energy variance $\langle\Delta H^2\rangle_{N_b}$ for each N_b.

Figure 3 shows the energy and energy variance of the variational wave functions obtained by the original MCSM and the SCG method in Sect.3.1. As N_b increases the energy-variance point moves smoothly and approaches the y-axis or variance zero. The fitted curves for these points are shown as red solid lines, and also approach the y-axis smoothly. The extrapolated energies, or y-intercepts of the fitted curves, agree quite well with the exact one, which is shown as a dashed line. The minimum variance of the SCG wave function is $\langle\Delta H^2\rangle_{N_b=100} = 0.54\text{MeV}^2$, which is smaller and gives a better approximation than the result of the original MCSM, $\langle\Delta H^2\rangle_{N_b=150} = 1.04\text{MeV}^2$. It means that the SCG method improves the accuracy of the MCSM wave function to a certain extent. Both the extrapolated energies of the original MCSM and the SCG agree with the exact energy quite well within a keV.

4. Summary

We reported the collaboration projects concerning the MCSM over the latest decade, including the introduction of Alphleet-1 and Alphleet-2 clusters and the recent code developments for utilizing state-of-the-art massively parallel computers. As the computational environment evolves, the code of the MCSM has been developed intermittently. In parallel, the framework of the MCSM has been extended such as the introduction of the conjugate gradient method and the energy-variance extrapolation. Currently we have finished the benchmark tests and start production runs on K computer under the SPIRE project. The recent achievements of this activity are seen in Refs.[1, 3, 10, 18, 19, 20].

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